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# Review of Numerical Methods

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# Numerical Solution to Differential Equations in CFD

**Classification of PDE**
- PDE type
  - Parabolic
  - Hyperbolic
  - Elliiptic
- Linear or Nonlinear
- Order of PDE
- Homogeneuos

**Boundary and initial conditions**
- fixed, fluxed, or mixed

**Choice of state variables**
- Primitive variables (pressure, velocity, density, ...)
- Non-primative
  - stream and vorticity functions
  - spectrum of primative variables

**Method of producing discrete equations from continuous conservation eqns**
- Finite Difference
- Finite Volume
- Weighted Residuals
  - Finite Element
  - Collocation / Spectral
- Boundary value ....

**Solution method for time evolution**
- Explicit
- Implicit
- Mixed

**Solution method for a given state**
- Direct substituion
- Matrix solution (Implicit method)
  - Direct inversion
  - Iterative (Successive Over Relaxation)
    - always necessary if nonlinear

**Meaning of computational points (Mesh or nonmesh)**
- Material movement thru mesh
  - Eulerian (spatial points)
  - Lagrangian (material points) SPH and Free Lagrangian
  - ALE (Arbitrary Lagrangian-Eulerian)
- Logical or Unstructured mesh
- Fixed connectivity or Variable connectivity: Free Lagrangian; SPH

**Choice of coordinates**
- rectangular
- curvilinear
  - cylindrical (2D: rz, r-theta)
  - spherical

**Order of solution (accuracy per cell or cycle)**
- Spatial
- Temporal

**Solution charateristics**
- Stability
- Consistancy
- Accuracy
- Efficiency
- Convergence and Convergence rates

# Introduction to Computational Fluid Dynamics

**Nomenclature**

**Notation** for partial derivatives

$$\frac{\partial u}{\partial x} \equiv u_x \qquad (\textbf{or } D_x u \textbf{ or } \partial_x u)$$

$$\frac{\partial^2 u}{\partial x \partial y} \equiv u_{xy} \qquad (\textbf{or } D_{xy} u \textbf{ or } \partial_{xy} u)$$

**Vector notation**

| | |
|---|---|
| a vector: | $\underline{u}, \vec{u}, \underset{\sim}{u}, \underset{\longrightarrow}{u}, \mathbf{u}$ |
| a tensor (2nd order) | $\underline{\underline{\tau}}, \vec{\vec{\tau}}, \underset{\sim}{\tau}, \underset{\Longrightarrow}{\tau}, \boldsymbol{\tau}$ |

components of a vector:

$$\begin{aligned} \mathbf{u} &= u_1\boldsymbol{\delta}_1 + u_2\boldsymbol{\delta}_2 + u_3\boldsymbol{\delta}_3 \\ &= \sum_{i=1}^{3} u_i \boldsymbol{\delta}_i \\ \mathbf{u} &= u_i\boldsymbol{\delta}_i \quad \text{using summation convention} \end{aligned}$$

unit tensor (also $\mathbf{I}$)

$$\boldsymbol{\delta} = \sum_{i=1}^{3} \boldsymbol{\delta}_i \cdot \boldsymbol{\delta}_i$$

$$\boldsymbol{\delta} = \delta_{ij}\boldsymbol{\delta}_i\boldsymbol{\delta}_j \quad \text{where} \quad \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

Kroneker delta

divergence $\qquad \nabla = \boldsymbol{\delta}_i \dfrac{\partial}{\partial x_i}$

Laplacian $\qquad \nabla^2 = \nabla \cdot \nabla = \dfrac{\partial}{\partial x_i^2}$

# Classification of Partial Differential Equations

**Order** of PDE: order of highest derivative in PDE

**Type:**

A general, 2nd order PDE:

$$a\,\partial_{xx}u + b\,\partial_{xy}u + c\,\partial_{yy}u + e = 0$$

**or**

$$a\,u_{xx}u + b\,u_{xy} + c\,u_{yy} + e = 0$$

where $a, b, c, d, e$ may be functions of $x, y, u, u_x, u_y$

then

| | | |
|---|---|---|
| **hyperbolic** if | $b^2 - 4ac > 0$ | (roots real & distinct) |
| | $u_{xx} - u_{yy} = f(u_x, u_y, x, y, u)$ | |
| **parabolic** if | $b^2 - 4ac = 0$ | (roots real & equal) |
| | $u_{xx} = f(u_x, u_y, x, y, u)$ | |
| **elliptic** if | $b^2 - 4ac < 0$ | (roots: complex) |
| | $u_{xx} + u_{yy} = f(u_x, u_y, x, y, u)$ | |

Classification not affected by nonsingular transformation of variables.

Each classification has different behavior and solution techniques.

**Linearity**

A PDE is **linear** if the principle of superposition holds:

if $u_1$ and $u_2$ are solutions to a given PDE,

then $a_1u_1 + a_2u_2$ is also a solution ($a_1$ and $a_2$ constants)

otherwise the PDE is **nonlinear**.

# Boundary and Initial Conditions

**consider**

$$u_{xx} + u_{yy} = 0$$

when integrated, the solution contains four unknowns. Naturally would specify $u(x, y)$ on four boundaries → **boundary conditions**

**consider**

$$u_t = u_{xx} + u_{yy} \qquad \text{(heat eqn.)}$$

$$u_{tt} = c^2 u_{xx} + c^2 u_{yy} \qquad \text{(wave eqn.)}$$

would require 5 and 6 prescribed conditions, but have only 4 boundaries → require 1 and 2 additional solutions at a prescribed time, typically $t = 0$ → **initial conditions**

**General form** of boundary conditions for $u(x, y)$

$$\alpha(x, y)u + \beta(x, y)u_n = \gamma(x, y)$$

where $u_n$ is the derivative of $u$ normal to boundary.

**Special forms**

$\gamma = 0$ : homogeneous b.c. (otherwise nonhomogeneous)

$\beta = 0$ : Dirichlet b.c. **or** specified $u$ b.c.

$\alpha = 0$ : Neumann b.c. **or** Flux b.c.

# Hyperbolic PDE

Two forms: $\phi_{\xi\xi} - \phi_{\eta\eta} = f_1(\phi_\xi, \phi_\eta, \phi, \xi, \eta)$ typical form

$\phi_{\xi\eta} = f_2(\phi_\xi, \phi_\eta, \phi, \xi, \eta)$ characteristic coordinate form

These can be shown to be equivalent through a coordinate transformation.

Hyperbolic (and parabolic) equations result from problems involving time as one independent variable and semi-infinite domain (time is unbounded). They require boundary and initial conditions.

Hyperbolic equations generally originate from vibration problems or from problems where discontinuities can persist in time (shock waves).

Analytic solutions of two independent variables often use the method of characteristics, which reduce the solution to solving ordinary differential equations.

Unlike elliptic and parabolic solutions, the influence of the domain on the solution at a particular point is limited in extent (see the following example).

**Example** Solve

$$u_{tt} = c^2 u_{xx} \qquad -\infty < x < +\infty$$

b.b. (1): $u(x,0) = f(x)$

b.c. (2): $u_t(x,0) = g(x)$

use the alternative form $u_{\xi\eta} = 0$ where

$$\xi = x - ct$$

$$\eta = x + ct$$

**Hyperbolic PDE** (cont.)

Integrate

$$u(\xi, \eta) = F_1(\eta) + F_2(\xi)$$

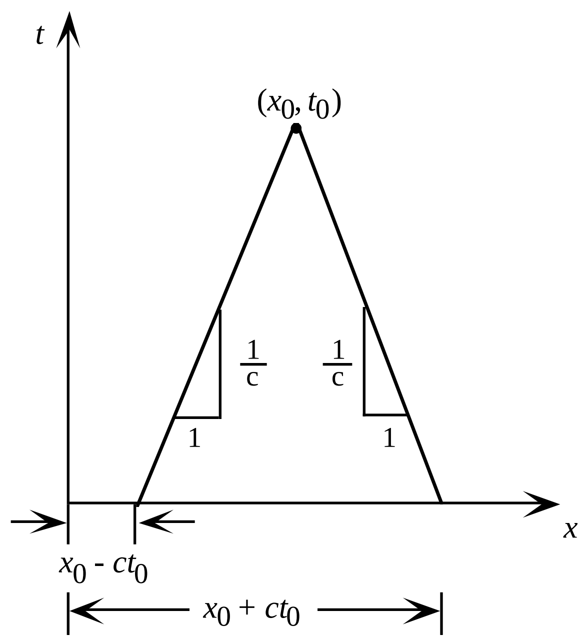
$$\textbf{or} \quad u(x,t) = F_1(x+ct) + F_2(x-ct)$$

b.c. (1): $f(x) = F_1(x) + F_2(x)$

b.c. (2): $g(x) = cF_1'(x) - cF_2'(x)$

$\Rightarrow u(x,t) = \frac{1}{2}\left[f(x+ct) - f(x-ct)\right] + \frac{1}{2c}\int_{x-ct}^{x+ct} g(\tau)d\tau$

**Note** solution at $(x_0, t_0)$ only depends on initial data: $x_0 - ct_0 \leq x \leq x_0 + ct_0$




- behavior characteristics of all hyperbolic equations

# Parabolic PDE

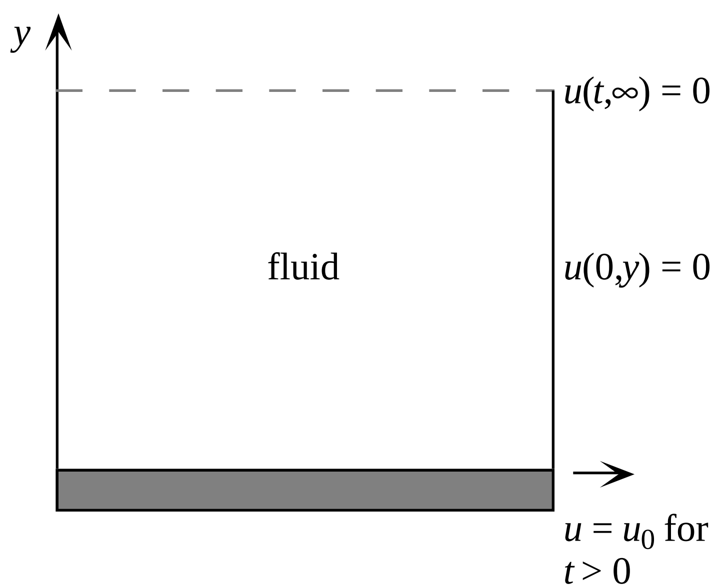
General Form: $\phi_{\xi\xi} = f(\phi_\xi, \phi_\eta, \phi, \xi, \eta)$

Parabolic equations result from diffusional processes that have time as one independent variable and a semi-infinite domain. They require initial and boundary conditions. They do not exhibit the limited zones of influence that hyperbolic equations have, i.e., the solution of a parabolic PDE at some time depends on the state in the physical domain at all earlier times.

**Example**. Rayleigh problem: viscous fluid set in motion by a uniformly moving flat plate.

$$u_t = \nu u_{yy} \quad \text{for} \quad 0 < y < \infty$$

$$\begin{array}{rl} \text{i.c.} & u(0,y) = 0 \\ \text{b.c. 1} & u(t,0) = u_0 \quad \text{for} \quad t > 0 \\ \text{b.c. 2} & u(t,\infty) = 0 \end{array}$$



**Parabolic PDE** (continued)

**Solve** by similarity solution. Introduce a change of variables (a guess) that may reduce the number of independent variables from 2 to 1. $\Rightarrow$ PDE $\rightarrow$ ODE.

$$\text{use} \qquad \eta = \frac{y}{2\sqrt{\nu t}} \Rightarrow \frac{\partial u(\eta)}{\partial t} = -\frac{y\nu}{4}(\nu t)^{3/2}\frac{\partial u}{\partial \eta}$$

$$\& \quad \frac{\partial^2 u(\eta)}{\partial y^2} = \frac{1}{4\nu t}\frac{\partial^2 u}{\partial \eta^2}$$

then PDE becomes

$$\frac{\partial^2 u}{\partial \eta^2} + \frac{y}{\sqrt{\nu t}}\frac{\partial u}{\partial \eta} = \frac{\partial^2 u}{\partial \eta^2} + 2\eta\frac{\partial u}{\partial \eta} = 0$$

same for boundary and initial conditions

$$\text{b.c. 1}: \qquad u(\eta = 0) = u_0$$

$$\text{i.c. \& b.c. 2}: \qquad u(\eta \rightarrow \infty) = 0$$

**Because** $t$ and $y$ do not appear in PDE or b.c. or i.c. then similarity solution worked.

**Integrate** ODE

$$\begin{aligned}
\frac{d}{d\eta}\frac{du}{d\eta} &= -2\eta\frac{du}{d\eta} \\
\ln\frac{du}{d\eta} &= -\eta^2 + c_1' \\
\frac{du}{d\eta} &= c_1 e^{-\eta^2} \\
\Rightarrow u &= \int c_1 e^{-\eta^2}\, d\eta + c_2
\end{aligned}$$

Apply b.c.

$$\begin{aligned}
u(\eta) &= u_0\left[1 - \frac{2}{\sqrt{\pi}}\int_0^{\eta} e^{-\eta^2}\, d\eta\right] \\
u(\eta) &= u_0\left[1 - \operatorname{erf}(\eta)\right]
\end{aligned}$$

# Elliptic PDEs

General form:

$$\phi_{\xi\xi} + \phi_{\eta\eta} = f\left(\phi_\xi, \phi_\eta, \xi, \eta, \phi\right)$$

are associated with **equilibrium** or steady state problems in a **bounded** domain.

The solution at any point in the domain depends on the boundary conditions at every point **or** a disturbance introduced at any point influences all other points in the domain.

Examples: Laplace's and Poisson's equation

$\nabla^2\phi = 0$ $\qquad$ $\nabla^2\phi = g$

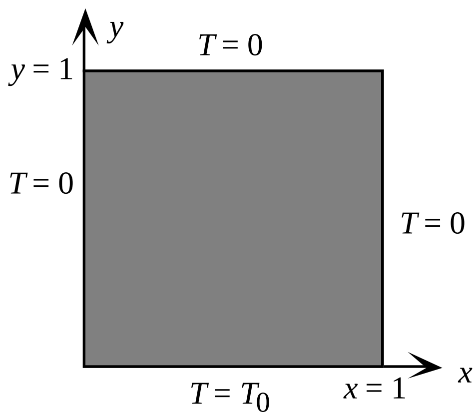
Solvable analytically only for simple geometries

**Example** Heat conduction in a block

$$\nabla^2 T = T_{xx} + T_{yy} = 0 \quad \text{for} \quad 0 \leq x \leq 1 \quad \text{and} \quad 0 \leq y \leq 1$$

$$T(0,y) = 0 \quad T(1,y) = 0$$

$$T(x,0) = T_0 \quad T(x,1) = 0$$




**Solve** by separation of variables: assume: $T(x,y) = X(x)Y(y)$

**then** $\qquad X'' + \alpha^2 X = 0 \qquad Y'' - \alpha^2 Y = 0$

$\qquad X(0) = 0$

$\qquad X(1) = 0 \qquad Y(1) = 0$

**solution** $\qquad X(x) = A\sin(\alpha x) \qquad Y(y) = c\sinh[\alpha(y-1)]$

**b.c.** $\qquad X(1) = 0 \Rightarrow \alpha = n\pi \qquad n = 1, 2, \ldots$

$$T(x,0) = T_0 \Rightarrow A_n = \tfrac{2T_0}{n\pi}\left[\tfrac{(-1)^n - 1}{\sinh(n\pi)}\right]$$

then $\qquad T(x,y) = \sum_{n=1}^{\infty} A_n \sin(n\pi x)\sinh[n\pi(y-1)]$

# Examples of PDEs

**1. 1st order wave equation** (hyperbolic)

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0 \qquad \textbf{or} \qquad u_t + cu_x = 0$$

Propagation of a wave at speed $c$. Note: different from 2nd order wave equation—equivalent to two coupled first-order wave equations.

**2. 2nd order wave equation** (hyperbolic)

$$\frac{\partial^2 y}{\partial t^2} - \alpha^2 \frac{\partial^2 y}{\partial x^2} = 0$$

Motion of a string.

**3. Burger's equation**

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} \qquad \textbf{or} \qquad u_t + uu_x = \nu u_{xx}$$

Nonlinear wave equation with diffusion.

Fluid flow with viscosity in 1D.

**4. Tricomi equation** (elliptic or hyperbolic)

$$yu_{xx} + u_{yy} = 0$$

describes steady state, inviscid, transonic flows in 2D

**5. Poisson's equation** (elliptic)

$$u_{xx} + u_{yy} = f(x, y)$$

Steady state heat conduction with a heat source in a solid.

Electric field in a region of charge.

If $f(y, x) = 0$, becomes Laplace equation.

**6. Advection-diffusion equation in 1D**

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = \alpha \frac{\partial^2 \phi}{\partial x^2}$$

Advection of passive scalar $\phi$ with velocity $u$ and with viscosity (or diffusion $\alpha$).

$\partial_t \phi = \alpha \partial_{xx} \phi$ is the unsteady heat or diffusion equation (parabolic).

**7. Helmholtz equation** (elliptic)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + k^2 u = 0$$

Governs the motion of time-dependent harmonic waves where $k$ is the frequency parameter.

# General Navier-Stokes Equations

Motion of a continuous medium is governed by classical mechanics (conservation of mass, momentum and energy) and thermodynamics.

Most general form of the conservation equations is in integral form (properties can be discontinuous).

**mass** $$\frac{d}{dt}\int_V \rho\, dV + \int_S \rho\mathbf{u}\cdot\mathbf{n}\, dS = 0$$

**momentum** $$\frac{d}{dt}\int_V \rho\mathbf{u}\, dV + \int_S \left[(\mathbf{n}\cdot\mathbf{u})\rho\mathbf{u} - \mathbf{n}\cdot\boldsymbol{\sigma}\right]\, dS = \int_V \rho\mathbf{f}\, dV$$

**total energy** $$\frac{d}{dt}\int_V \rho E\, dV + \int_S \mathbf{n}\cdot\left[\rho E\mathbf{u} - \boldsymbol{\sigma}\cdot\mathbf{u} + \mathbf{q}\right]\, dS = \int_V \rho\mathbf{f}\cdot\mathbf{u}\, dV$$

$V$ & $S$ are the stationary volume and surface

$\mathbf{n}$ is the normal to surface $S$

$t$ – time

$\rho$ – density

$\mathbf{u}$ – velocity

$\mathbf{f}$ – external force per volume

$\mathbf{q}$ – heat flux

$\boldsymbol{\sigma}$ – stress tensor

traction $= \mathbf{n}\cdot\boldsymbol{\sigma}$ (area)

$E$ – total energy per mass

$E = I + \frac{1}{2}u^2$

$\uparrow$ internal energy

**Navier-Stokes Equations** (continued)

If properties are continuous and sufficiently differentiable, then integral form $\Rightarrow$ conservative differential form:

use Gauss Divergence thru

$$\int\limits_V \nabla \cdot \boldsymbol{\nu} \, dV = \int\limits_S \mathbf{n} \cdot \boldsymbol{\nu} \, dS$$

**mass** $$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

**momentum** $$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u} - \boldsymbol{\sigma}) = \rho \mathbf{f}$$

**total energy** $$\frac{\partial}{\partial t} \rho E + \nabla \cdot (\rho E \mathbf{u} - \boldsymbol{\sigma} \cdot \mathbf{u} + \mathbf{q}) = \rho \mathbf{f} \cdot \mathbf{u}$$

Alternative energy form (internal energy equation)

$$\rho \frac{De}{Dt} - \boldsymbol{\sigma} : \nabla \mathbf{u} + \nabla \cdot \mathbf{q} = 0$$ assuming $\boldsymbol{\sigma}$ symmetric

**Not** in conservative form!

where

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla$$ substantial or material derivative

Often the stress tensor $\boldsymbol{\sigma}$ is divided into an isotropic component, the thermodynamic pressure $p$, and a deviatoric stress tensor $\boldsymbol{\tau}$

$$\boldsymbol{\sigma} = -p \boldsymbol{\delta} + \boldsymbol{\tau}$$

**Note** these conservation equations hold for all materials but must have constitutive equations to be useful.

**Navier Stokes Equations** (continued)

Use Newton's Law of Viscosity with $\kappa = 0$ and Fourier's Law of Heat Conduction

then $\quad \boldsymbol{\tau} = \mu \left[\dot{\boldsymbol{\gamma}} - \frac{2}{3}(\nabla \cdot \mathbf{u})\boldsymbol{\delta}\right]$

Then the conservation equation for momentum becomes

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \rho \mathbf{f} + \nabla \cdot \mu \left[\dot{\boldsymbol{\gamma}} - \frac{2}{3}(\nabla \cdot \mathbf{u})\boldsymbol{\delta}\right]$$

Navier-Stokes equation

The corresponding internal energy equation is

$$\rho \frac{De}{Dt} + p\nabla \cdot \mathbf{u} = \Phi - \nabla \cdot \mathbf{q}$$
$$\Phi = \boldsymbol{\tau} : \nabla u = -\frac{2}{3}\mu(\nabla \cdot \mathbf{u})^2 + \frac{1}{2}\mu \dot{\boldsymbol{\gamma}} : \dot{\boldsymbol{\gamma}}$$

$\Phi$, dissipation function, is the rate at which mechanical energy is converted into heat.

Alternative energy equation in terms of $T$

$$\rho C_p \frac{DT}{Dt} = k\nabla^2 T + \Phi \qquad \text{often} \quad \nu = \frac{k}{\rho C_p}$$

with $\quad K = \text{const.}$

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla$$

# Constitutive Relationships

— Relate state variables to fluxes

$$(\rho, \mathbf{u}, E, I) \quad \text{to} \quad (p, \mathbf{q}, \boldsymbol{\sigma})$$

— Are material dependent, both in functionality and in the specification of values for the parameters in the constitutive equation.

— Are usually empirical in origin—but can be derived theoretically in some cases.

**Examples**

**Equation of State (EOS)** $\quad p(\rho, e)$ **or** $p(\rho, T)$

(assumes equilibrium thermodynamics)

$$p = (\gamma - 1)\rho e$$

Ideal or gamma-law gas

**Fourier's Law of Heat Conduction**

$$\mathbf{q} = -k\nabla T$$

$T$ is the temperature

and

$k$ is the thermal conductivity

**Newton's Law of Viscosity**

$$\boldsymbol{\tau} = \left(\kappa - \frac{2}{3}\mu\right)(\nabla \cdot \mathbf{u})\boldsymbol{\delta} + \mu\dot{\boldsymbol{\gamma}}$$

$\mu$ - shear viscosity

$k$ - bulk or dilatational viscosity

$\kappa = 0$ for simple fluids (monotonic gases)

$\boldsymbol{\delta}$ - identity tensor

$\dot{\boldsymbol{\gamma}} = [\nabla\mathbf{u} + (\nabla\mathbf{u})^{+}]$

# Limiting Forms of the Navier Stokes Equations

**Incompressible** $(\nabla \cdot \mathbf{u} = 0)$ Note: this **does not** mean uniform density.

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \delta \mathbf{f} + \nabla \cdot (\mu \dot{\boldsymbol{\gamma}})$$

$$\rho C_p \frac{DT}{Dt} = K \nabla^2 T + \frac{1}{2} \mu \dot{\boldsymbol{\gamma}} : \dot{\boldsymbol{\gamma}}$$

const $k$ & $\mu$

**Creeping flow** (Inertia neglected or small $N_{Re} = \frac{D\mu}{\nu}$)

$$\frac{Du}{Dt} \rightarrow \frac{\partial u}{\partial t}$$

(note: not steady state)

**Constant Viscosity**

$$\nabla \cdot (\mu \dot{\boldsymbol{\gamma}}) \rightarrow \mu \nabla \cdot \dot{\boldsymbol{\gamma}}$$

**Invisid** $(\mu = 0)$

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \rho \mathbf{f}$$

$$\rho C_p \frac{DT}{Dt} = k \nabla^2 T$$

**Burger's Equation** $f = 0$, incompressible

$p = \text{const}$, 1D flow $u(t, x)$

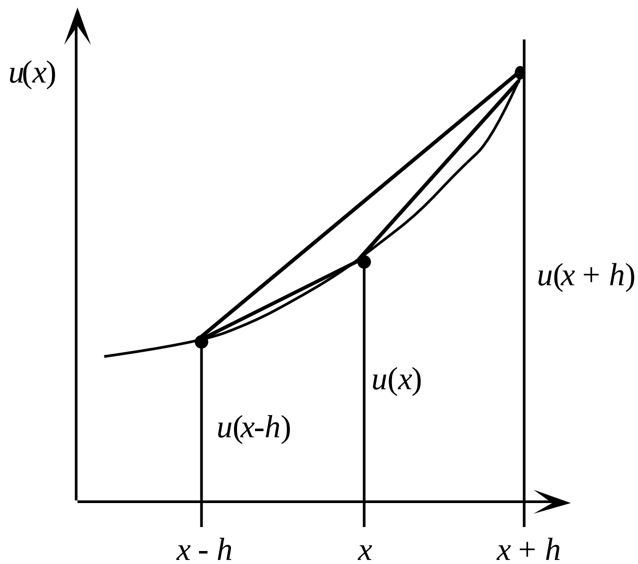
$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$$

$\vdots$ and many others

# Difference Approximations for Derivatives

**Recall** the Taylor Series

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^2 f'''}{3!}(x) + \underbrace{O(h^4)}_{\substack{\text{(does not} \\ \text{indicate size} \\ \text{—just rate)}}}$$




**then**

$$u(x+h) = u(x) + hu'(x) + \frac{1}{2}h^2u''(x) + \frac{1}{6}h^3u'''(x) + O(h^4) \tag{1}$$

$$u(x-h) = u(x) - hu'(x) + \frac{1}{2}h^2u''(x) - \frac{1}{6}h^3u'''(x) + O(h^4) \tag{2}$$

**add** (1) and (2)

$$u(x+h) + u(x-h) = 2u(x) + h^2u''(x) + O(h^4)$$

**solve** for $u''(x)$

$$u''(x) = \left(\frac{d^2u}{dx^2}\right)_{x=x} = \frac{1}{h^2}\left\{u(x+h) - 2u(x) + u(x-h)\right\} + O(h^2)$$

**subtract** (1) and (2) (3)

$$u(x+h) - u(x-h) = 2hu'(x) + O(h^3)$$

**Difference approximations** (continued)

**solve** for $u'(x)$

$$u'(x) = \frac{1}{2h}\{u(x+h) - u(x-h)\} + O(h^2) \tag{4}$$

Equations (3) and (4) represent central-difference approximations of the derivatives, and both have errors of $\mathbf{O}(h^2)$

**solve** (1) and (2) for $u'(x)$ directly

$$\begin{aligned} u'(x) &= \frac{1}{h}\{u(x+h) - u(x)\} + O(h) && \text{forward difference} \\ u'(x) &= \frac{1}{h}\{u(x) - u(x-h)\} + O(h) && \text{backward difference} \end{aligned}$$

Note: that these have error of $O(h)$ where the central difference approximations have $O(h^2)$.

**General Form** $(-1 \le \alpha \le 1)$

$$u'(x) \approx \frac{(1-\alpha)u(x+h) + 2\alpha u(x) - (1+\alpha)u(x-h)}{2h}$$

The error is $-\frac{\alpha h}{2}u''(x) - \frac{h^2}{6}u'''(x)$

| | | |
|---|---|---|
| for | $\alpha = 0$ | centered |
| | $\alpha = 1$ | backward |
| | $\alpha = -1$ | forward |

$\Rightarrow$ Error is only $h^2$ for $\alpha$ exactly equal to 0.

Using the Taylor expansion, one can find higher order approximations, for example

$$u'(x) = \frac{-u(x+2h) + 8u(x+h) - 8u(x-h) + u(x-2h)}{12h} + O(h^2)$$

In general: "Higher order — reach farther"

## Finite-Difference Method

Finite-difference method replaces the **continuous** problem domain by a **discrete** or finite difference mesh or grid.

$$\textbf{Define} \qquad x_i \equiv i\Delta x \,, \qquad x_{i+1} = (i+1)\Delta x$$

$$u_i \equiv u(x_i)$$

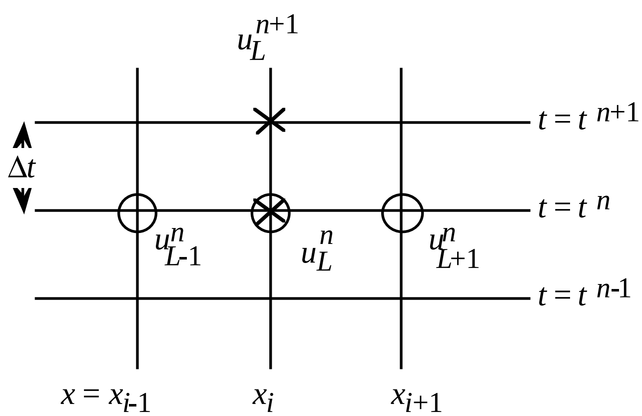
In a similar manner, the time domain is discretized:

$$t^n \equiv n\,\Delta t$$

$$\text{for } u(t,x) : \qquad u_i^n \equiv u(n\Delta t, x_i)$$

Finite-difference method replaces the derivatives in a PDE with finite approximations.

**Examples** with $u(t,x)$




$$\textbf{forward} \qquad \left(\frac{\partial u}{\partial t}\right)_{\substack{t=t^n \\ x=x_i}} \approx \frac{u_i^{n+1} - u_i^n}{\Delta t} \qquad \times \text{ - above}$$

$$\textbf{central} \qquad \left(\frac{\partial^2 u}{\partial x^2}\right)_{\substack{t=t^n \\ x=x_i}} \approx \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \qquad \bigcirc \text{ - above}$$

**Finite-Difference Method** (continued)

**Example** (continued)

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \Rightarrow \frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}$$

Assume all values at $t^n$ known, solve for unknown $u_i^{n+1}$

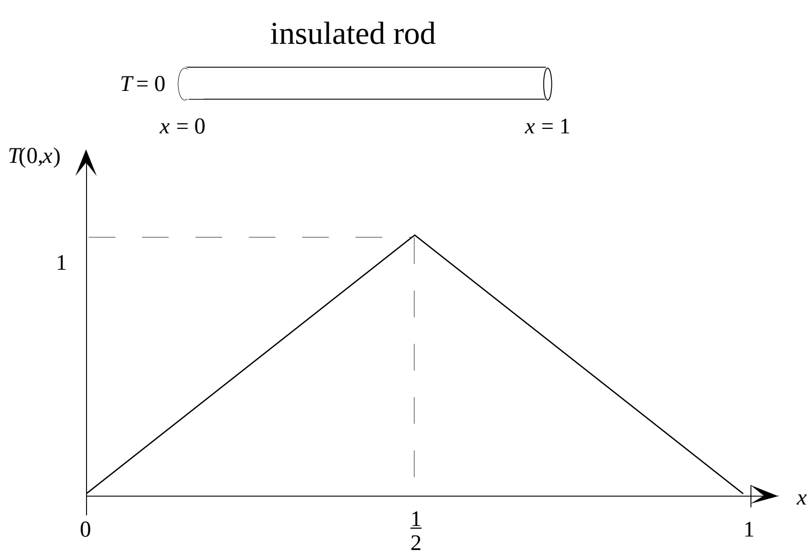
$$u_i^{n+1} = r\, u_{i+1}^n + (1-2r)u_i^n + r\, u_{i-1}^n$$
$$\text{where} \qquad r = \frac{\Delta t}{\Delta x^2}$$

Therefore, given boundary values and initial values, $u_i^{n+1}$ can be calculated for all future times at all positions.

**Example**

$$\textbf{solve} \quad \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} \qquad\qquad \text{parabolic, heat conduction in 1D.}$$
$$\textbf{i.c.} \quad T(0,x) = \begin{cases} 2x & 0 \le x \le \frac{1}{2} \\ 2(1-x) & \frac{1}{2} \le x \le 1 \end{cases}$$
$$\textbf{b.c. 1} \quad T(t,0) = 0$$
$$\textbf{b.c. 2} \quad T(t,1) = 0$$

take $\left.\begin{array}{l} \Delta x = \frac{1}{10} \\ \Delta t = \frac{1}{10000} \end{array}\right\} r = \frac{1}{10}$



**Finite Difference Method** (continued)

solution $T_i^{n+1} = \frac{1}{10}\left(T_{i-1}^n + 8T_i^n + T_{i+1}^n\right)$

| | **i =** | **0** | **1** | **2** | **3** | **4** | **5** |
|---|---|---|---|---|---|---|---|
| | $\mathbf{x_i}$ = | **0** | **0.1** | **0.2** | **0.3** | **0.4** | **0.5** |
| **n** | **t** | | | | | | |
| **0** | **0** | 0 | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 |
| **1** | **0.001** | 0 | 0.2 | 0.4 | 0.6 | 0.8 | 0.96 |
| **2** | **0.002** | 0 | 0.2 | 0.4 | 0.6 | 0.7960 | 0.9280 |
| **3** | **0.003** | 0 | 0.2 | 0.4 | 0.5996 | 0.7896 | 0.9016 |
| **10** | **0.01** | 0 | 0.1996 | 0.3968 | 0.5822 | 0.7281 | 0.7867 |
| **20** | **0.02** | 0 | 0.1938 | 0.3781 | 0.5373 | 0.6486 | 0.6891 |

$$u_5^1 = \frac{1}{10}\left\{0.8 + (8 \times 1) + 0.8\right\} = 0.9600$$

$$u_4^2 = \frac{1}{10}\left\{0.6 + (8 \times 0.8) + 0.96\right\} = 0.7960$$

$$u_1^2 = \frac{1}{10}\left\{0 + (8 \times 0.2) + 0.4\right\} = 0.2$$

unchanged!

Analytical solution

$$T(t,x) = \frac{8}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\left(\sin\frac{1}{2}n\pi\right)(\sin n\pi x)\, e^{-n^2\pi^2 t}$$

**Example** Heat Conduction

Comparison of Finite difference and analytical solution at $x = 0.3$

| $t$ | FD | Analytical | Difference | % error |
|---|---|---|---|---|
| 0.005 | 0.5971 | 0.5966 | 0.0005 | 0.08 |
| 0.01 | 0.5822 | 0.5799 | 0.0023 | 0.4 |
| 0.02 | 0.5373 | 0.5334 | 0.0039 | 0.7 |
| 0.10 | 0.2472 | 0.2444 | 0.0028 | 1.1 |

A similar comparison at $x = 0.5$ shows errors of 2.3, 1.6, 1.2, 1.2 respectively $\Rightarrow$ Discontinuities in initial data lead to larger errors. Method is accurate to $O(\Delta t)$ if the initial data has derivatives that are continuous, otherwise decreases.

**Example** redo last problem but with the $\Delta t$ larger.

take: $\Delta x = \frac{1}{10}$ as before, $\Delta t = \frac{5}{1000}$ so $r = \frac{\Delta t}{\Delta x^2} = 0.5$

then $u_i^{n+1} = \frac{1}{2}\left(u_{i-1}^n + u_{i+1}^n\right)$

| | | **x = 0.1** | **0.2** | **0.3** | **0.4** | **0.5** | **0.6** |
|---|---|---|---|---|---|---|---|
| **t =** | **0.0** | 0.2000 | 0.4000 | 0.6000 | 0.8000 | 1.000 | 0.8000 |
| | **0.005** | " | " | " | " | 0.8000 | 0.8000 |
| | **0.010** | " | " | " | 0.7000 | 0.8000 | 0.7000 |
| | **0.015** | " | " | 0.5500 | 0.7000 | 0.7000 | 0.7000 |
| | **0.020** | " | 0.3750 | 0.5500 | 0.6250 | 0.7000 | 0.6250 |
| | ⋮ | | | | | | |
| | **0.100** | 0.0949 | 0.1717 | 0.2484 | 0.2778 | 0.3071 | 0.2778 |

**and**

| $t$ | FD ($x = 0.3$) | analytical | Difference | % error |
|---|---|---|---|---|
| 0.005 | 0.6000 | 0.5966 | 0.0034 | 0.57 |
| 0.01 | 0.6000 | 0.5799 | 0.0201 | 3.5 |
| 0.02 | 0.5500 | 0.5334 | 0.0166 | 3.1 |
| 0.1 | 0.2484 | 0.2444 | 0.0040 | 1.6 |

**Example** increase $\Delta t$ even more.

**take** $\Delta x = \frac{1}{10}$ as before, $\Delta t = \frac{1}{100}$, $r = 1.0$

| | **x =** | **0.1** | **0.2** | **0.3** | **0.4** | **0.5** |
|---|---|---|---|---|---|---|
| **t =** | **0.0** | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 |
| | **0.01** | " | " | " | " | 0.6 |
| | **0.02** | " | " | " | 0.4 | 1.0 |
| | **0.03** | " | " | 0.2 | 1.2 | −0.2 |
| | **0.04** | " | 0.0 | 1.4 | −1.2 | 2.6 |

using $u_L^{n+1} = u_{i-1}^n - u_i^n + u_{i+1}^n$

What's wrong? Fourier or von Neumann analysis shows that difference expression is **stable** if

$$0 < r \leq \frac{1}{2} \qquad \text{where} \quad r = \frac{\Delta t}{\Delta x^2}$$

(see next page)

In general, finite difference approximations of

(parabolic) $\quad \dfrac{\partial u}{\partial t} = \alpha \dfrac{\partial^2 u}{\partial t^2}$ $\quad$ has stability restrictions based on $\quad \alpha \dfrac{\Delta t}{\Delta x^2}$

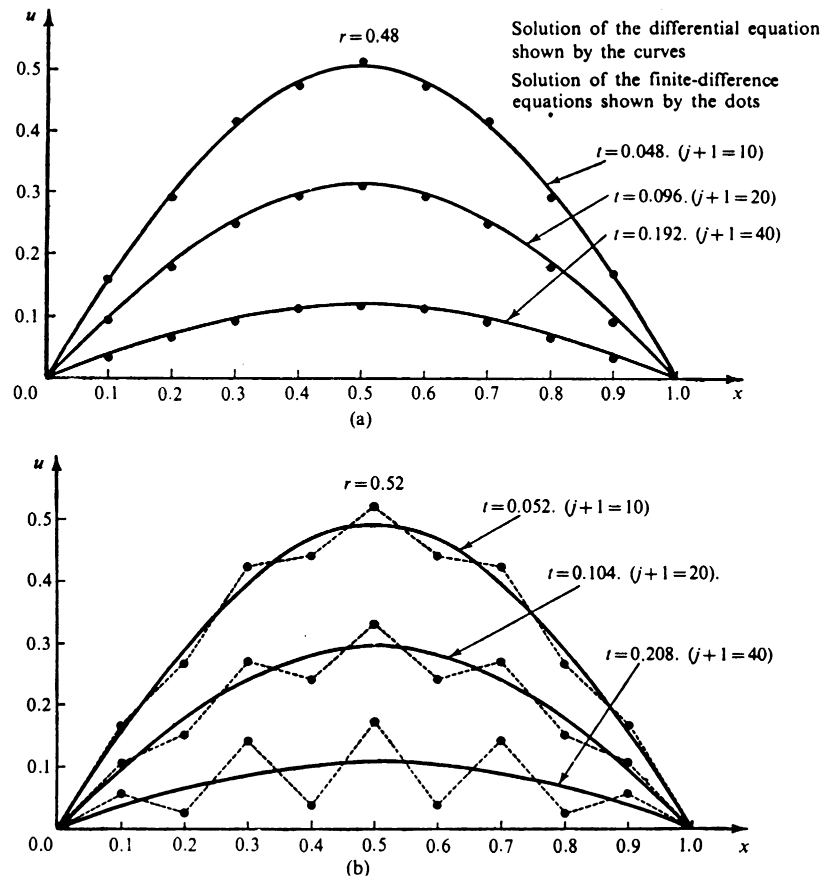
**and**

(hyperbolic) $\quad \dfrac{\partial u}{\partial t} = -c \dfrac{\partial u}{\partial x}$ $\quad$ has restrictions based on $\quad c \dfrac{\Delta t}{\Delta x}$ ,

the Courant-Friedrichs-Lewy (CFL) condition

**and**

(mixed) $\quad \dfrac{\partial u}{\partial t} + c \dfrac{\partial u}{\partial t} = \alpha \dfrac{\partial^2 u}{\partial x^2}$ $\quad$ has restrictions on both.




**Top figure for r = 0.48**

**Bottom figure for r = 0.52**

Comparison of the solution around the turning point for stability, r = 1/2.

# Important Concepts in Numerical Methods

**Truncation error** is the difference between the PDE and the equivalent finite difference expression (FDE).

**Example** for the heat conduction equation

$$\underbrace{\frac{\partial u}{\partial t} - \alpha \frac{\partial^2 u}{\partial x^2}}_{\text{PDE}} = \underbrace{\frac{u_j^{n+1} - u_j^n}{\Delta t} - \frac{\alpha}{\Delta x^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right)}_{\text{FDE}}$$

$$+ \underbrace{\left[-\frac{\partial^2 u}{\partial t^2}\Big|_{n,j} \frac{\Delta t}{2} + \alpha \frac{\partial^4 u}{\partial x^4}\Big|_{n,j} \frac{\Delta x^2}{12} + \ldots\right]}_{\text{T.E. of } 0(\Delta t, \Delta x^2)}$$

### Discretization and Round-Off Errors

Round-off errors occur because of limited precision on computers. In some FDEs, round-off errors are proportional to $\Delta x$, then refining the mesh may reduce the truncation error but increase the round-off error.

In the absence of round-off errors, discretization error is the difference between the solution of the PDE and the FDE. The discretization error is caused by the truncation error, plus any errors introduced by the boundary and initial conditions.

**Important Concepts** (continued)

**Stability**

A stable numerical process limits amplification of all components of the initial conditions. Stability is a subtle concept that is difficult to establish analytically. The Fourier analysis perturbs the FDE at all frequency components and an expression is locally stable if all components remain bounded. Locally stable is also called weakly stable.

**Example**

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} = \frac{\alpha}{\Delta x^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right)$$

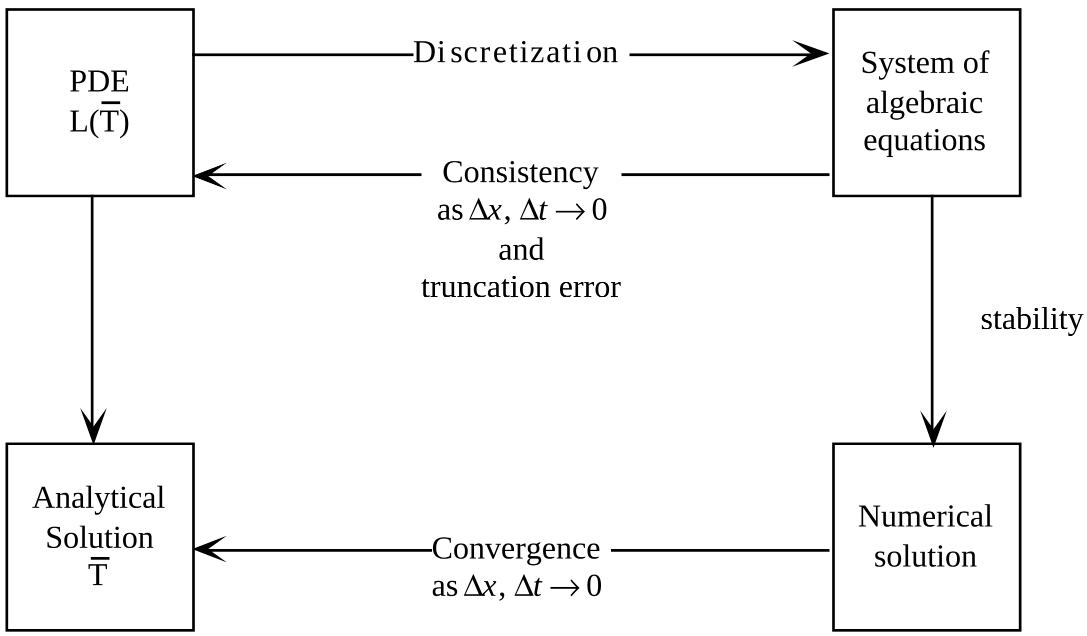
has a truncation error of $O(\Delta t^2, \Delta x^2)$ but is unconditionally unstable for any $\Delta t, \Delta x$.

**Consistency**

An FDE that is **consistent** or **compatible** with the PDE is one which the truncation error goes to zero as $\Delta t$ and $\Delta x$ go to zero.

**Convergence**

An FDE is convergent is the solution to the FDE tends to the solution of the PDE as $\Delta t$ and $\Delta x$ go to zero.




Relationship between concepts

**Important Concepts** (continued)

**Well or properly posed problem**

A problem is properly posed if:

i) The solution is unique if it exists.

ii) The solution depends continuously on the initial data.

iii) A solution always exists for initial data that is arbitrarily close to initial data for which no solution exists. (A continuous approximation to a boundary condition that is discontinuous.)

Comment: often nonlinear PDEs are ill posed.

**Desire**: Well-posed computational solution, too.

**Lax's equivalence theorem**

Given a properly posed linear, initial value problem and a linear finite difference that satisfies the consistency conditions,

Stability is a necessary and sufficient condition for convergence.

The reason why we often accept a stable solution as an accurate solution.

**For the Navier-Stokes equations:**

— not possible to demonstrate convergence directly.

— can show methods are consistent.

— can usually show linearized equations are stable.

Therefore, Lax theorem tends to provide a necessary, rather than sufficient, condition for convergence for the Navier-Stokes equations.

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